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ON EULERIAN MODELING OF MICROCHANNEL GAS FLOWS CLOSING HIGHER STATISTICAL MOMENTS OF MOLECULE VELOCITY

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ABSTRACT

High pressure gradient driven micro-channel flow modelling with very the high ratios of absolute pressure and temperature (see Agrawal et al. 2005 [1]) define the difference between physical and computational results using continuum approaches (see Maurer et al. 2003, Durst et al. 2006, Dongari et al. 2008 [3,4,8]). In the present paper this deviation of the computational results is explained by the statistical correlation of the molecular number density and the single molecule velocity inside a compressible gas flow. Classical solutions of Navier-Stokes equations do not satisfy the physical conditions of compressible, dilute molecular flows (see Brenner 2005, Greenshields and Reese 2007, Mizzi et al. 2008 [2, 6, 9]). Furthermore the consistent entropy production and the comparison between macroscopic physical values and the molecular diffusion closure are shown. Finally the computational results using this statistical model are compared with algebraic solutions verifying the thermodynamic consistence of the present statistical moment closure model.

NOMENCLATURE

- a sonic speed [m/s]
- d_m molecule diameter [m]
- *e* internal energy [J/kg]
- *h* enthalpy [J/kg]
- k_B Boltzmann constant (= $1.38065 \cdot 10^{-23} J/K$)
- m molecule mass [kg]

- *p* pressure [*Pa*]
- s entropy [J/(kgK)]
- *t* time coordinate [*s*]
- u_i fluid velocity [m]
- v specific volume $[m^3/kg]$
- x_i space coordinate [*m*]
- D diffusivity coefficient $[m^2/s]$
- *E* deviation tensor [*Pa*]
- *M* mole mass [kg/mol]
- R_0 general gas constant (= 8.31447 J/(mol K))
- *T* absolute temperature [*T*]
- γ heat capacity ratio [-]
- ζ molecule velocity variance $[m^2/s^2]$
- κ degrees of freedom [-]
- μ viscosity [*Pas*]
- ξ_i molecule velocity [m/s]
- ρ desity $[kg/m^3]$
- σ molecule velocity standard deviation [m/s]
- Φ diffusion tensor [*Pa*]
- Pr Prandtl number [-]
- Sc Schmidt number [-]

INTRODUCTION

Inside a compressible gas flow clouds of molecules move through a pre-defined flow-volume geometry inside a dilute gas

n molecule number density $\left[1/m^3\right]$

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flow. The single molecules diffuse with different molecule velocities ξ_i and a mean number density \bar{n} (Knudsen 1909, Grad 1949 [5, 10]). Based on the tree conservation equations of mass, momentum and energy the transport equation of molecule clouds are defined with the molecule number density *n* and the molecule velocity ξ_i by the time-averaged form of the equation array:

$$\frac{\partial}{\partial t}\left(\bar{n}\right) + \frac{\partial}{\partial x_{j}}\left(\overline{n\xi_{j}}\right) = 0 \tag{1}$$

$$\frac{\partial}{\partial t} \left(\overline{n\xi_i} \right) + \frac{\partial}{\partial x_j} \left(\overline{n\xi_i} \overline{\xi_j} \right) = 0 \tag{2}$$

$$\frac{\partial}{\partial t} \left(\frac{\overline{n}}{2} \xi_i \xi_i \right) + \frac{\partial}{\partial x_j} \left(\frac{\overline{n}}{2} \xi_i \xi_i \xi_j \right) = 0 \quad . \tag{3}$$

The conservation is satisfied by the neglecting time devivative of the integrated form. Computing mass flux and momentum of the present gas flow the mean velocity is defined with a numberdensity weighted averaging scheme by the ratio:

$$\tilde{\xi}_j = \frac{\mathrm{E}(n\xi_j)}{\mathrm{E}(\bar{n})} = \frac{\overline{n\xi_j}}{\bar{n}} \quad . \tag{4}$$

By that the continuity equation is written in the averaging form as follows:

$$\frac{\partial}{\partial t}\left(\bar{n}\right) + \frac{\partial}{\partial x_{j}}\left(\bar{n}\tilde{\xi}_{j}\right) = 0 \quad . \tag{5}$$

Multiplied with the mass of a single molecule this relation has the same form as the classical mass conservation.

NUMBER DENSITY CORRELATIONS

Modelling the molecule number density/velocity correlation with following number density and momentum gradient dependencies

$$\overline{n'\xi_j} = -D\frac{\partial\bar{n}}{\partial x_j} \quad \Rightarrow \quad \bar{\xi}_j = \tilde{\xi}_j + \frac{D}{\bar{n}}\frac{\partial\bar{n}}{\partial x_j} \tag{6}$$

the statistical moment closure produces the transport equation of the molecular momentum. Transforming the time-averaged convection term following triple correlation has to be closed additionally.

$$\overline{n'\xi_i\xi_j} = -D\left(\frac{\partial}{\partial x_j}\overline{n\xi_i} + \frac{\partial}{\partial x_i}\overline{n\xi_j}\right)$$
(7)

The additional diffusion coefficient D defines the molecular motion not resolved by the mean mass flux, the macroscopic convection [7].

Developing the velocity correlation

$$\widetilde{\xi_{i}''}\widetilde{\xi_{j}''} = \frac{2\zeta}{\kappa}\delta_{ij} + \frac{D^{2}}{\bar{n}^{2}}\left[\frac{\partial\bar{n}}{\partial x_{i}}\frac{\partial\bar{n}}{\partial x_{j}} - \frac{1}{\kappa}\frac{\partial\bar{n}}{\partial x_{k}}\frac{\partial\bar{n}}{\partial x_{k}}\delta_{ij}\right] \\ -D\left[\frac{\partial\tilde{\xi}_{j}}{\partial x_{i}} + \frac{\partial\tilde{\xi}_{i}}{\partial x_{j}} - \frac{2}{\kappa}\frac{\partial\tilde{\xi}_{k}}{\partial x_{k}}\delta_{ij}\right]$$
(8)

and substituting its trace with 2ζ the specific momentum transport equation get additional source terms depending on mean molecule velocity and mean number density gradients:

$$\frac{\partial}{\partial t} \left(\bar{n} \tilde{\xi}_{i} \right) + \frac{\partial}{\partial x_{j}} \left(\bar{n} \tilde{\xi}_{i} \tilde{\xi}_{j} \right) =$$

$$- \frac{\partial}{\partial x_{i}} \left[\frac{\bar{n}}{\kappa} \widetilde{\xi}_{k}^{\prime\prime} \widetilde{\xi}_{k}^{\prime\prime} \right]$$

$$+ \frac{\partial}{\partial x_{j}} \left[D \bar{n} \left(\frac{\partial \tilde{\xi}_{j}}{\partial x_{i}} + \frac{\partial \tilde{\xi}_{i}}{\partial x_{j}} - \frac{2}{\kappa} \frac{\partial \tilde{\xi}_{k}}{\partial x_{k}} \delta_{ij} \right) \right]$$

$$- \frac{\partial}{\partial x_{j}} \left[\frac{D^{2}}{\bar{n}} \left(\frac{\partial \bar{n}}{\partial x_{i}} \frac{\partial \bar{n}}{\partial x_{j}} - \frac{1}{\kappa} \frac{\partial \bar{n}}{\partial x_{k}} \frac{\partial \bar{n}}{\partial x_{k}} \delta_{ij} \right) \right] .$$
(9)

These additional terms explain momentum variation depending on microscopic physical values, whose have tho be interpreted with macroscopic forces by a transformation from the hardsphere molecule cloud diffusion approach to the macroscopic thermodynamics of dissipative systems.

Interpreting the number density weighted by the molecular mass as density, the diffusion coefficient *D* as momentum diffusion coefficient (Sc = 1) and the weighted-averaged molecule velocity as the mean gas velocity macroscopic values are defined by molecular quantities in the following way (App. A). So the product of the trace of the velocity correlation tensor, the density ρ and the inverse molecular degrees of freedom $1/\kappa$ defines the pressure of a dilute and thermodynamically ideal gas.

$$\rho = m\bar{n} \qquad \mu = m\bar{n}D \\
u_i = \tilde{\xi}_i \qquad p = m\frac{\bar{n}}{\kappa}\widetilde{\xi''_k\xi''_k} \qquad (10)$$

These approximations help parallelizing microscopic molecular approaches and macroscopic physical views. With the definition of the mean kinetic molecular energy

$$\zeta = \frac{1}{2} \widetilde{\xi_k''} \widetilde{\xi_k''} \tag{11}$$

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the specific pressure is proportional with this energy:

$$\frac{p}{\rho} = \frac{1}{\kappa} \widetilde{\xi_k''} \widetilde{\xi_k''} = \frac{\gamma - 1}{2} \widetilde{\xi_k''} \widetilde{\xi_k''} = (\gamma - 1) \zeta \quad . \tag{12}$$

In this way macroscopic values are interpreted as derviatives of molecular diffusion and kinetics.

HIGHER MOLECULE VELOCITY MOMENT CLOSURE

Developing the kinetic energy transport equation of the mean velocity multiplying the momentum equation with a weighted-averaged velocity term

$$\frac{\partial}{\partial t} \left(\frac{\bar{n}}{2} \tilde{\xi}_i \tilde{\xi}_i \right) + \frac{\partial}{\partial x_j} \left(\frac{\bar{n}}{2} \tilde{\xi}_i \tilde{\xi}_i \tilde{\xi}_j \right) = -\tilde{\xi}_j \frac{\partial}{\partial x_j} \left(\bar{n} \widetilde{\xi_i'' \xi_j''} \right)$$
(13)

the difference of this equation and the time-averaged energy transport produces an equation of the velocity variance:

$$\frac{\partial}{\partial t} \left(\frac{\bar{n}}{2} \widetilde{\xi_i''} \widetilde{\xi_i''} \right) + \frac{\partial}{\partial x_j} \left(\frac{\bar{n}}{2} \widetilde{\xi_i''} \widetilde{\xi_i''} \widetilde{\xi_j} \right) =$$

$$-\bar{n} \widetilde{\xi_i''} \widetilde{\xi_j''} \frac{\partial \widetilde{\xi_i}}{\partial x_j} - \frac{\partial}{\partial x_j} \left(\frac{\bar{n}}{2} \widetilde{\xi_i''} \widetilde{\xi_i''} \widetilde{\xi_j''} \right)$$

$$(14)$$

Developing the third statistical moment the time-averaged form has to be closed. Using the following approximation

$$\overline{\xi_i'\xi_j'\xi_k'} = \frac{D}{\bar{n}} \left[\frac{\partial}{\partial x_i} \left(\bar{n}\Phi_{jk} \right) + \frac{\partial}{\partial x_j} \left(\bar{n}\Phi_{ik} \right) + \frac{\partial}{\partial x_k} \left(\bar{n}\Phi_{ij} \right) \right]$$
(15)

with a function of the deviation tensor

$$\Phi_{ij} = -2\frac{\mu}{\rho} \underbrace{\left(\frac{\partial \tilde{\xi}_i}{\partial x_j} + \frac{\partial \tilde{\xi}_j}{\partial x_i} - \frac{2}{3} \frac{\partial \tilde{\xi}_k}{\partial x_k} \delta_{ij}\right)}_{E_{ij}} \qquad (16)$$

the transport equation of the molecular energy ζ

$$\frac{\partial}{\partial t}(\bar{n}\zeta) + \underbrace{\frac{\partial}{\partial x_{j}}\left(\bar{n}\zeta\tilde{\xi}_{j}\right)}_{\text{convection}} \qquad (17)$$

$$= \underbrace{\frac{\partial}{\partial x_{j}}\left(D\bar{n}\frac{\kappa+2}{\kappa}\frac{\partial\zeta}{\partial x_{j}}\right)}_{\text{diffusion}} \underbrace{-\bar{n}\frac{2}{\kappa}\zeta\frac{\partial\tilde{\xi}_{k}}{\partial x_{k}}}_{\text{compression dissipation}} = \overline{n}\Phi_{ij}\frac{\partial\tilde{\xi}_{i}}{\partial x_{j}}$$



consists of the relation between convection, diffusion, compression, dissipation and production terms.

COMPRESSIBLE DYNAMICS AND THERMODYNAMIC CONSISTENCE

In the definition of the sonic speed the molecule velocity standard deviation σ , what is proportional with the square-root of the internal energy *e*, is proportional with the speed of sound:

$$a^{2} = \frac{\mathrm{d}p}{\mathrm{d}\rho} = \gamma \frac{p}{\rho} = \gamma (\gamma - 1) \zeta \tag{18}$$

$$\Rightarrow \sigma = \sqrt{\frac{2}{\kappa}\zeta} = \frac{a}{\sqrt{\gamma}} \quad . \tag{19}$$

With the theory of *Clausius and Duhem* the change of internal energy in an isentropic case is different from the case, if the entropy *s* is increasing:

$$de = Tds - pdv \Leftrightarrow \rho \dot{\zeta} = \rho T \dot{s} - p\rho \dot{v} \quad . \tag{20}$$

With the definition of the specific volume $v = 1/\rho$ the timederivate of the kinetic energy of a molecule cloud is resulting:

$$\dot{\rho}\zeta + \rho\dot{\zeta} = \rho T \dot{s} - \frac{\dot{v}}{v}(p + \rho\zeta)$$
$$= \bar{n}T \dot{s} - \bar{n}\underbrace{\frac{\kappa + 2}{\kappa}}_{=\gamma}\zeta \frac{\partial \tilde{\xi}_k}{\partial x_k} \quad . \tag{21}$$

Transforming the developed transport equation of the velocity variance (eq. 14)

$$\frac{\mathrm{d}}{\mathrm{d}t}(\bar{n}\zeta) = \frac{\partial}{\partial t}(\bar{n}\zeta) + \tilde{\xi}_{j}\frac{\partial}{\partial x_{j}}(\bar{n}\zeta)$$

$$= -\bar{n}\widetilde{\xi_{i}''\xi_{j}''}\frac{\partial\tilde{\xi}_{i}}{\partial x_{j}} - \frac{\partial}{\partial x_{j}}\left(\frac{\bar{n}}{2}\widetilde{\xi_{i}''\xi_{i}''\xi_{j}''}\right) - \bar{n}\zeta\frac{\partial\tilde{\xi}_{j}}{\partial x_{j}} (22)$$

and substituting the molecule velocity variance derive the change of entropy is developed. To provide the thermodynamic consistence of this statistical method the entropy production is gener-

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ated:

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$$iT\dot{s} = \bar{n}\frac{\kappa+2}{\kappa}\zeta\frac{\partial\tilde{\xi}_{k}}{\partial x_{k}} + \frac{d}{dt}(\bar{n}\zeta)$$

$$= \frac{\partial}{\partial x_{j}}\left(\frac{1}{\kappa}\frac{D^{3}}{\bar{n}^{2}}\frac{\partial\bar{n}}{\partial x_{i}}\frac{\partial\bar{n}}{\partial x_{i}}\frac{\partial\bar{n}}{\partial x_{j}}\right) - \bar{n}\Phi_{ij}\frac{\partial\tilde{\xi}_{i}}{\partial x_{j}}$$

$$+ \frac{\partial}{\partial x_{j}}\left(D\bar{n}\frac{\kappa+2}{\kappa}\frac{\partial\zeta}{\partial x_{j}} - D^{2}\frac{\kappa+2}{\kappa}\frac{\partial\tilde{\xi}_{i}}{\partial x_{i}}\frac{\partial\bar{n}}{\partial x_{j}}\right) \quad (23)$$

and becomes positive for all thermodynamic changes as prescribed by the second law of thermodynamics.

GOVERNING TRANSPORT EQUATIONS

Finally the thermodynamically consistent set of conservation equations with the adiabatic exponent $\gamma = c_p/c_v = (\kappa + 2)/\kappa$ results for compressible flows:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_j) = 0$$

$$\frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_j} (\rho u_i u_j) = -\frac{\partial p}{\partial x_i}$$

$$+ \frac{\partial}{\partial x_j} [2\mu E_{ij}]$$

$$- \frac{\partial}{\partial x_j} \left[\frac{\mu^2}{\rho^3} \left(\frac{\partial \rho}{\partial x_i} \frac{\partial \rho}{\partial x_j} - \frac{\gamma - 1}{2} \frac{\partial \rho}{\partial x_k} \frac{\partial \rho}{\partial x_k} \delta_{ij} \right) \right]$$
(25)

$$\frac{\partial}{\partial t}(\rho\zeta) + \frac{\partial}{\partial x_j}(\rho\zeta u_j) = -\rho\zeta(\gamma - 1)\frac{\partial u_j}{\partial x_j} + 2\mu E_{ij}\frac{\partial u_i}{\partial x_j} + \frac{\partial}{\partial x_j}\left(\gamma\mu\frac{\partial\zeta}{\partial x_j}\right)$$
(26)

$$-\frac{\partial}{\partial x_{j}}\left[\left(\gamma\mu\frac{\partial u_{i}}{\partial x_{i}}-\frac{\gamma-1}{2}\frac{\mu^{2}}{\rho^{3}}\frac{\partial\rho}{\partial x_{i}}\frac{\partial\rho}{\partial x_{i}}\right)\frac{\mu}{\rho^{2}}\frac{\partial\rho}{\partial x_{j}}\right]$$

$$2m\sqrt{(\gamma-1)\zeta}$$
(27)

with
$$\mu = \frac{2\pi i}{3d_m^2} \sqrt{\frac{(1-1)^2}{\pi^3}}$$
 (27)

and
$$E_{ij} = \frac{1}{2} \left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \right)$$
 (28)

The viscosity μ defining parameters are the specific molecular kinetic energy ζ , the molecule mass *m* and the molecule diameter d_m . Neglecting the direct influence of pressure gradients in the upper equations, the effective *Prandtl number* is Pr < 1. Therefore the specific enthalpy would be defined by the formulation $h = \gamma \zeta$.



FIGURE 1. MEAN FLUID VELOCITY PROFILES

RESULTS AND DISCUSSION

The validation case is given by the reference case of a heated laminar channel flow [4] with an inlet Reynolds number of 1137. The fluid medium is air with $\gamma = 1.4$ by a temperature of 300*K* and an atmospheric pressure of 101325*Pa*. The channel height is H = 41mm and the inlet velocity is 0.5m/s. The wall temperature is given with 1000*K*. Typically following values of molecule mass and diameter are obtained $m = 4,80 \cdot 10^{-26}kg$ and $d_m = 3,06 \cdot 10^{-10}m$. The gravity works across the flow orientation in negative y-direction.

The results of the *present model* are compared with the kinetic diffusion theory (Pr=1) and the computational results of a diffusion-source model with additional diffusion source terms of Durst et al. [4]. The velocity profiles of the present model match the profiles of the diffusion-source model very good especially in the channel center. Density and temperature profiles agree with the diffusion-source model inside the shear layer near the wall. In the channel center the diffusion-source model results are closer to the kinetic theory results with a compressible approximation for dilute gases with Pr=1. So the heat transfer increase at the channel center is higher than shown in the diffusion-source model with additional source terms for that effect. The results of following models are compared: the present model (solid line), the kinetic theory (dashed line) and the diffusion source model (dots). Shown are the profiles of axial velocity, absolute temperature, fluid density and viscosity at the positions $x \in \{0.08, 0.2, 0.8, 1.6\}.$

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FIGURE 2. MEAN FLUID TEMPERATURE PROFILES



FIGURE 3. MEAN FLUID DENSITY PROFILES

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FIGURE 4. MEAN FLUID VISCOSITY PROFILES

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Appendix A: Equivalence of macroscopic and molecular values

	· ·
macroscopic	molecular
value	value
u _i	$\widetilde{\xi}_i$
$\zeta = e - h_0$	$\frac{1}{2}\widetilde{\xi_i''\xi_i''}$
$h - h_0$	$\left(\frac{1}{2} + \frac{1}{\kappa}\right)\widetilde{\xi_i''\xi_i''}$
R_0/M	k_B/m
γ	$1+2/\kappa$
C_{V}	$\kappa/2 \cdot k_B/m$
c_p	$(1+\kappa/2)k_B/m$
Т	$m/(\kappa k_B)\widetilde{\xi_i''\xi_i''}$
ρ	mī
\bar{c}	$\sqrt{8\widetilde{\xi_i''}\widetilde{\xi_i''}/(\pi\kappa)}$
$D=\mu/ ho$	$rac{2}{3ar{n}d_m^2}\sqrt{rac{(\gamma-1)\zeta}{\pi^3}}$
λ	$1/(\sqrt{2}\pi\bar{n}d_m^2)$
а	$rac{\kappa+2}{\kappa^2}\widetilde{\xi_i''\xi_i''}$

TABLE 1. PAIRS OF EQUIVALENT VALUES